## Claims:

I(We) claim:

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5 1. An isotopically enriched N-substituted piperazine acetic acid compound of the formula:

, or a salt thereof, comprising one or more heavy atom isotopes, wherein;

X is O or S;

Y is a straight chain or branched C1-C6 alkyl group or a straight chain or branched C1-C6 alkyl ether group wherein the carbon atoms of the alkyl group or alkyl ether group each independently comprise linked hydrogen, deuterium or fluorine atoms;

each Z is independently hydrogen, deuterium, fluorine, chlorine, bromine, iodine, an amino acid side chain, a straight chain or branched C1-C6 alkyl group that may optionally contain a substituted or unsubstituted aryl group wherein the carbon atoms of the alkyl and aryl groups each independently comprise linked hydrogen, deuterium or fluorine atoms, a straight chain or branched C1-C6 alkyl ether group that may optionally contain a substituted or unsubstituted aryl group wherein the carbon atoms of the alkyl and aryl groups each independently comprise linked hydrogen, deuterium or fluorine atoms or a straight chain or branched C1-C6 alkoxy group that may optionally contain a substituted or unsubstituted aryl group wherein the carbon atoms of the alkyl and aryl groups each independently comprise linked hydrogen, deuterium or fluorine atoms.

- 25 2. The compound of claim 1, wherein the N-substituted piperazine acetic acid is isotopically enriched with two or more heavy atom isotopes.
  - 3. The compound of claim 1, wherein the N-substituted piperazine acetic acid is isotopically enriched with three or more heavy atom isotopes.

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- 4. The compound of claim 1, wherein the N-substituted piperazine acetic acid is isotopically enriched with four or more heavy atom isotopes.
- 5 5. The compound of claim 1, wherein the heavy atom isotopes are each independently <sup>18</sup>O, <sup>15</sup>N or <sup>13</sup>C, but not deuterium.
  - 6. The compound of claim 1, wherein each Z is independently hydrogen, fluorine, chlorine, bromine or iodine.
  - 7. The compound of claim 1, wherein each Z is independently hydrogen, methyl or methoxy.
  - 8. The compound of claim 1, wherein Y is methyl, ethyl, *n*-propyl, isopropyl, *n*-butyl, isobutyl, *sec*-butyl or *tert*-butyl.
  - 9. The compound of claim 1, wherein X is  $^{16}O$  or  $^{18}O$ .
  - 10. The compound of claim 1, wherein each nitrogen atom of the piperazine ring is independently  $^{14}N$  or  $^{15}N$ .
  - 11. The compound of claim 1 of the formula:

wherein

X is O or S;

each C\* is independently <sup>12</sup>C or <sup>13</sup>C;

Y is a straight chain or branched C1-C6 alkyl group or a straight chain or branched

C1-C6 alkyl ether group wherein the carbon atoms of the alkyl group or alkyl ether group each independently comprise linked hydrogen, deuterium or fluorine atoms;

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each Z is independently hydrogen, deuterium, fluorine, chlorine, bromine, iodine, an amino acid side chain, a straight chain or branched C1-C6 alkyl group that may optionally contain a substituted or unsubstituted aryl group wherein the carbon atoms of the alkyl and aryl groups each independently comprise linked hydrogen, deuterium or fluorine atoms, a straight chain or branched C1-C6 alkyl ether group that may optionally contain a substituted or unsubstituted aryl group wherein the carbon atoms of the alkyl and aryl groups each independently comprise linked hydrogen, deuterium or fluorine atoms or a straight chain or branched C1-C6 alkoxy group that may optionally contain a substituted or unsubstituted aryl group wherein the carbon atoms of the alkyl and aryl groups each independently comprise linked hydrogen, deuterium or fluorine atoms.

12. The compound of claim 1 of the formula:

$$-N = \frac{13}{13}C = \frac{18}{18}OH = \frac{15}{18}N = \frac{15}{18}N$$

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- 13. The compound of claim 12, wherein the compound is a zwitterion, mono-TFA salt, a mono-HCl salt, a bis-TFA salt or a bis-HCl salt.
- The compound of claim 12, wherein each incorporated heavy atom isotope is present in at
  least 80 percent isotopic purity.
  - 15. The compound of claim 12, wherein each incorporated heavy atom isotope is present in at least 93 percent isotopic purity.

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- 16. The compound of claim 12, wherein each incorporated heavy atom isotope is present in at least 96 percent isotopic purity.
- 17. The compound of claim 1, wherein the N-substituted piperazine acetic acid is a mono-TFA
  5 salt, a mono-HCl salt, a bis-HCl salt or a bis-TFA salt.
  - 18. The compound of claim 1, wherein each incorporated heavy atom isotope is present in at least 80 percent isotopic purity.
- 19. The compound of claim 1, wherein each incorporated heavy atom isotope is present in at least 93 percent isotopic purity.
  - 20. The compound of claim 1, wherein each incorporated heavy atom isotope is present in at least 96 percent isotopic purity.
  - 21. The compound of claim 12, wherein the compound is a carboxylate anion.
  - 22. The compound of claim 1, wherein the compound is a carboxylate anion.